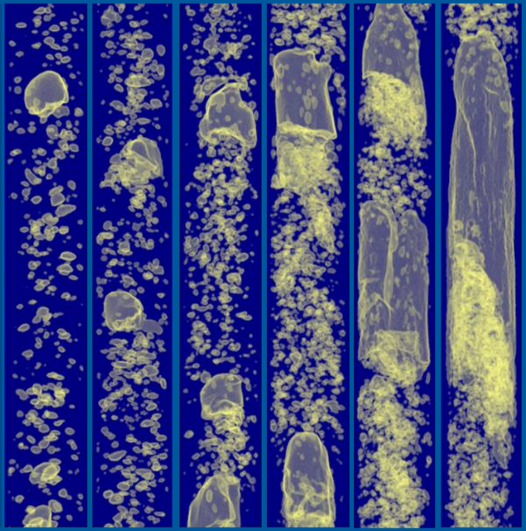
SKM DPG Conference, 28. September 2021


Einsatz bildgebender Messverfahren und numerischer Modellierungswerkzeuge für die Verbesserung der Energieeffizienz industrieller Mehrphasenprozesse

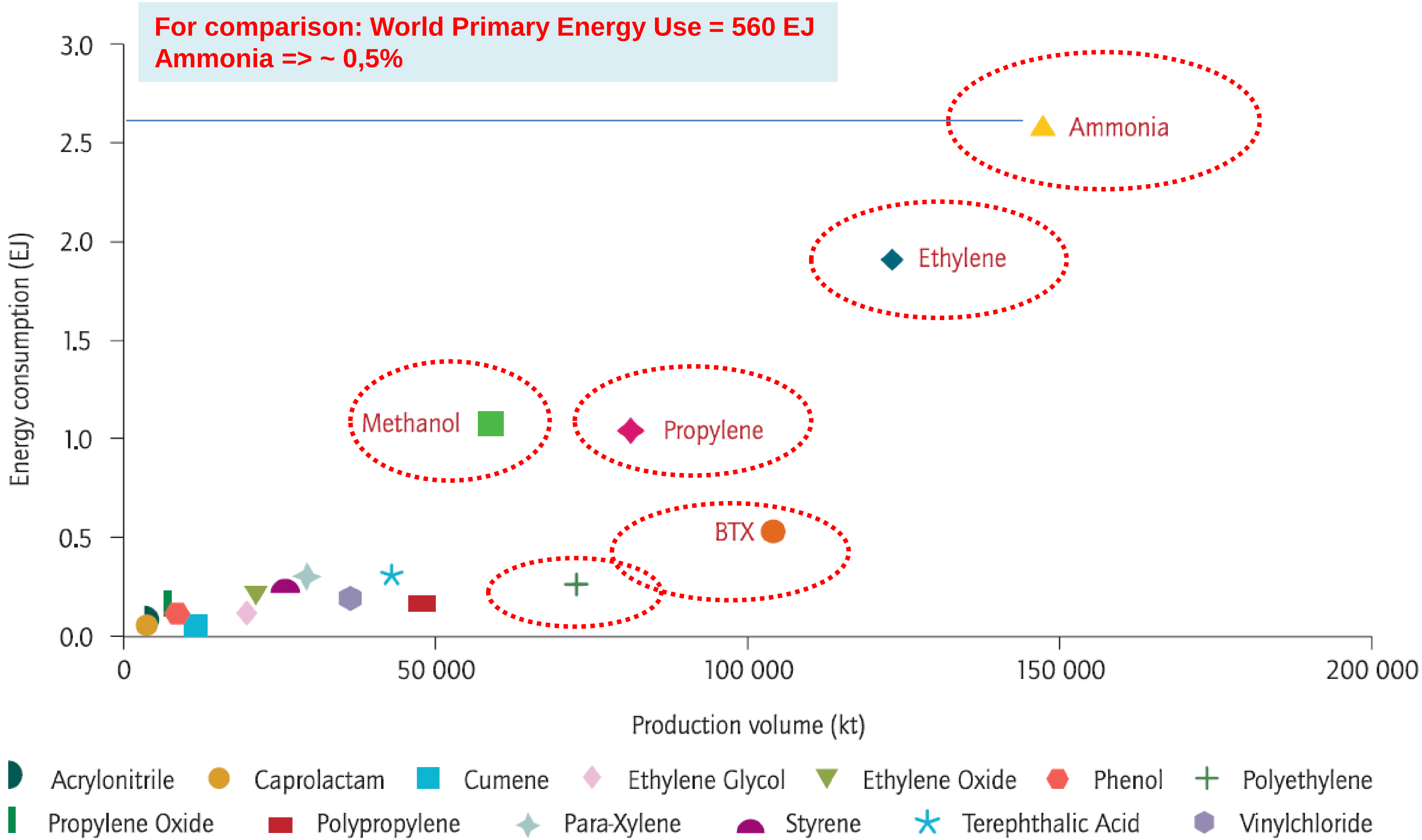
U. Hampel

HZDR
HELMHOLTZ ZENTRUM DRESDEN ROSSENDORF

Energy Consumption in Different Sectors

Total primary energy consumption in Germany 2018: 13.1 EJ

Energy Intensive Chemicals



Chemical Processes – Unit Operations

Reaction

Leverage:
- Optimal Process Design and Control
- Intensification
- Catalysts

Space-Time Yield
Selectivity

Downstream processing

Leverage:
- Optimal Design
- Flow Control
- Intensification

Separation Efficiency

Feedstock

Educts

Products
Side-Poducts
Educts

Wanted Product(s)

Energy

Heat (Process Steam)

Heat (Process Steam)

Heat (Process Steam)

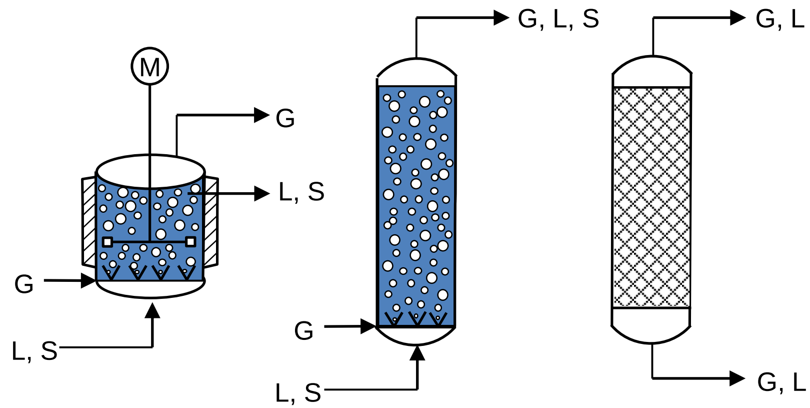
Heat Management

www.wikipedia.de

Chemical Processes – Unit Operations

90% of all chemical products are being produced in multiphase reactors

Acylation	$ArH + R{-}C({=}O)Cl \longrightarrow Ar{-}C({=}O){-}R + HCl$
Carbonylation	$R{-}OH + CO \rightarrow R{-}COOH$
Oxidative carbonylation	$R{-}NH_2 + CO + O_2 \rightarrow R{-}NHCOO{-}R + H_2O$
Dehydration	$R{-}OH \rightarrow R{=}CH_2 + H_2O$
Halogenation	$Ar{-}R + X_2 \rightarrow Ar{-}R'X\ (X = Cl_2, F_2, Br_2)$
Hydroformylation	${-}CH{=}CH{-} + CO + H_2 \longrightarrow CH_2{-}CH_2{-}C({=}O)H$
Hydrogenation	$R{-}CHO + H_2 \rightarrow RCH{-}OH$
Hydroxylation	${-}CH{=}CH{-} + O_2 \longrightarrow CH(OH){-}CH(OH)$
Nitration	$ArH \xrightarrow[H_2SO_4]{HNO_3} Ar{-}NO_2$
Oxidation	$Ar{-}R + O_2 \rightarrow Ar{-}R'OOH$



M. P. Dudukovic, Frontiers in Reactor Engineering, Science 325, 698, **2009**.

J. Hagen, Technische Katalyse, Wiley, **1996**.

The World of Multiphase Thermal Fluid Mechanics

Continuity equation

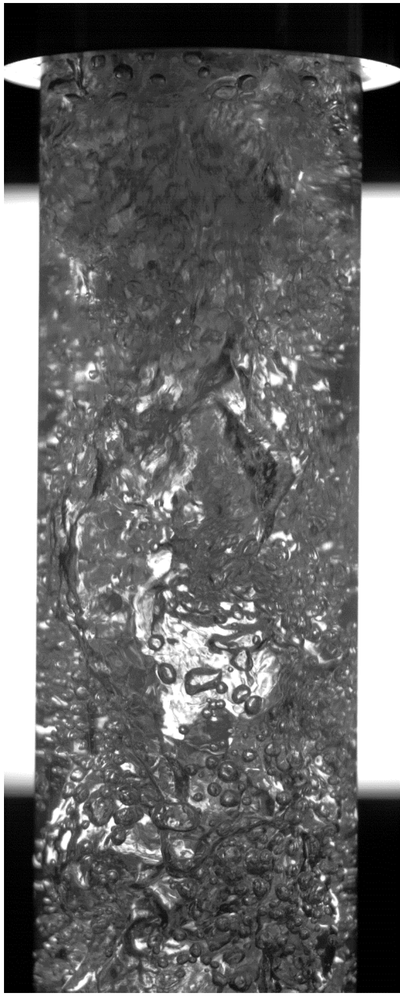
$$\frac{\partial \rho}{\partial t} + \nabla \cdot \boldsymbol{u} = 0$$

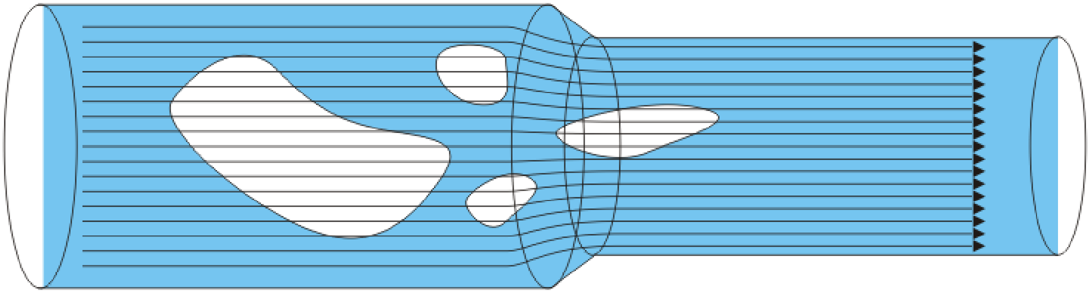
Momentum equation

$$\rho \left[\frac{\partial \boldsymbol{u}}{\partial t} + (\boldsymbol{u} \cdot \nabla \boldsymbol{u}) \right] = -\nabla p + \mu \Delta \boldsymbol{u} + f$$

Energy equation

$$\rho c_p \left[\frac{\partial T(\boldsymbol{r},t)}{\partial t} + (\boldsymbol{u}(\boldsymbol{r},t) \cdot \nabla T(\boldsymbol{r},t)) \right] = \lambda \Delta T(\boldsymbol{r},t) + q(\boldsymbol{r},t)$$





An Typical Setup for Multiphase CFD

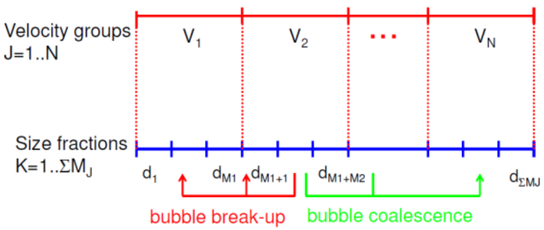
- Bubble forces (momentum exchange)

> 🕮 Lucas et al.; *Nucl. Eng. Des.*; **2016**

Bubble force	Model
drag	Ishii and Zuber (1979)
lift	Tomiyama (2002)
wall	Hosokawa (2002)
turb. disp.	Burns (2004)
virt. mass	$C_v = 1/2$

- Velocity groups (MUSIG model)

> 🕮 Krepper et al.; *Nucl. Eng. Des.*; **2008**



- SST turbulence model and BIT

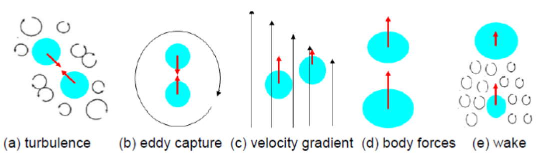
> 🕮 Ma et al.; *Phys. Rev. Fluids*; **2017**

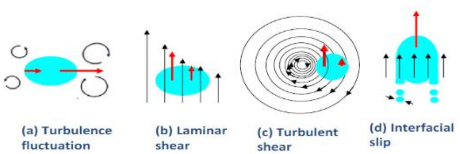
$$C_1 = 0.184 \cdot \mathrm{Re}^{0.229}$$

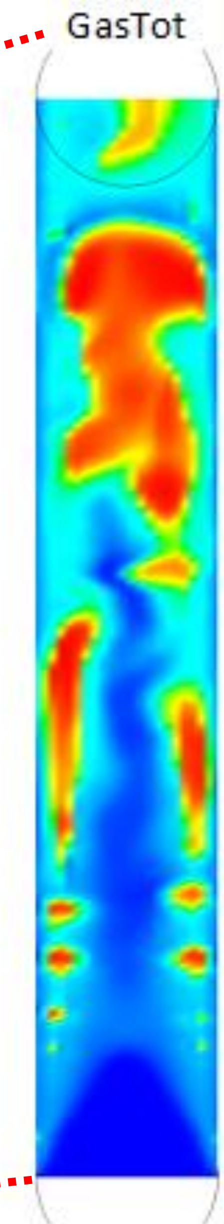
$$C_{\varepsilon B} = 0.3 \cdot C_D$$

- Coalescence and breakup

> 🕮 Liao et al.; *Chem. Eng. Sci.*; **2015**



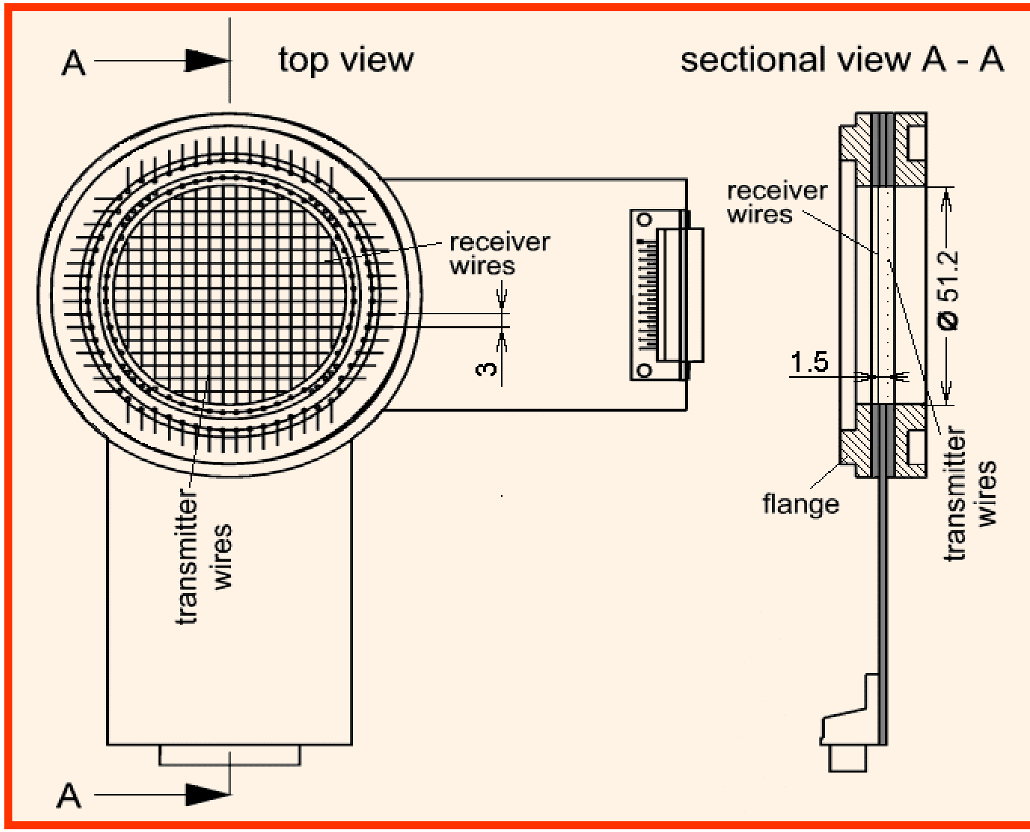




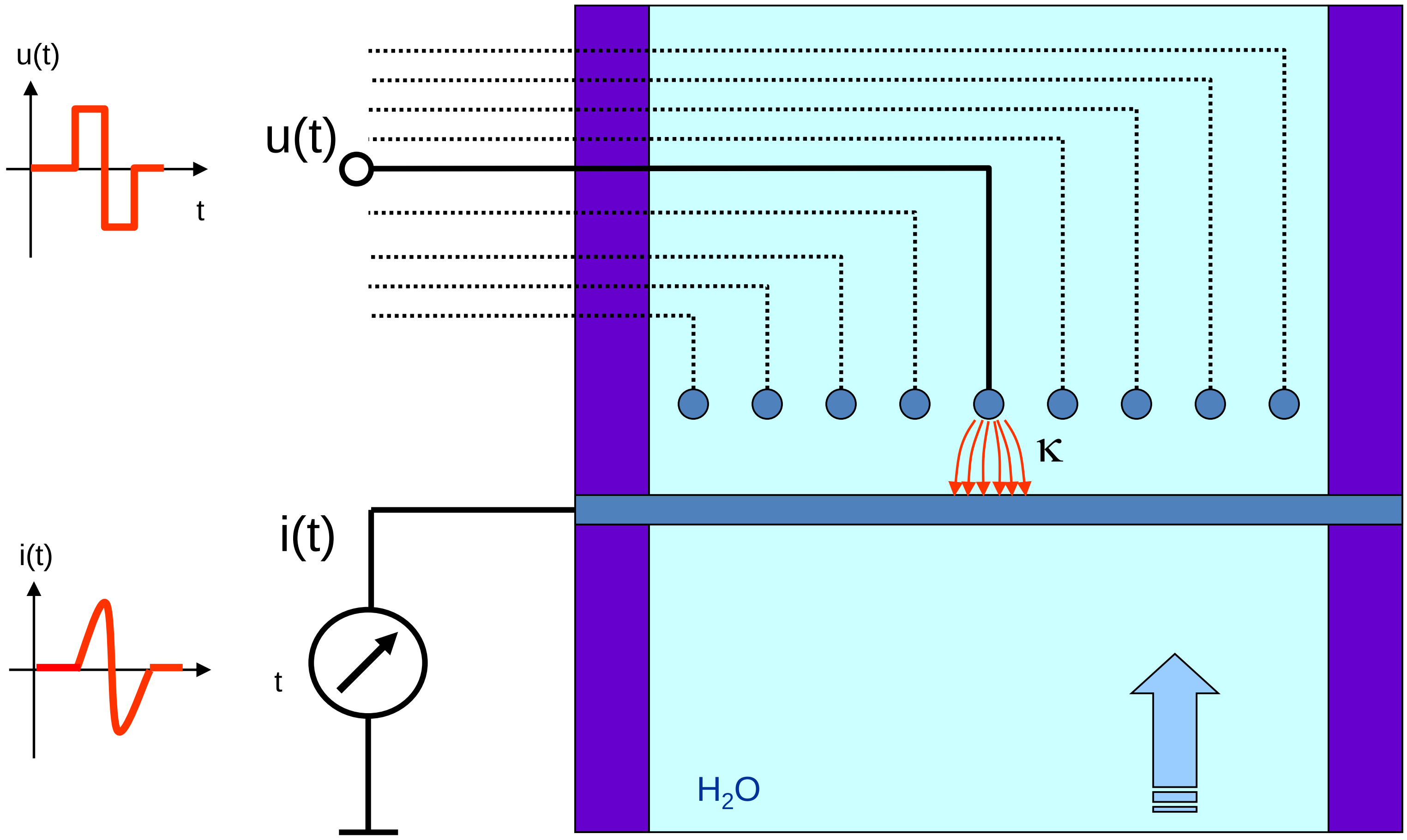
DRESDEN concept

Multiphase flow analysis with wire-mesh sensors

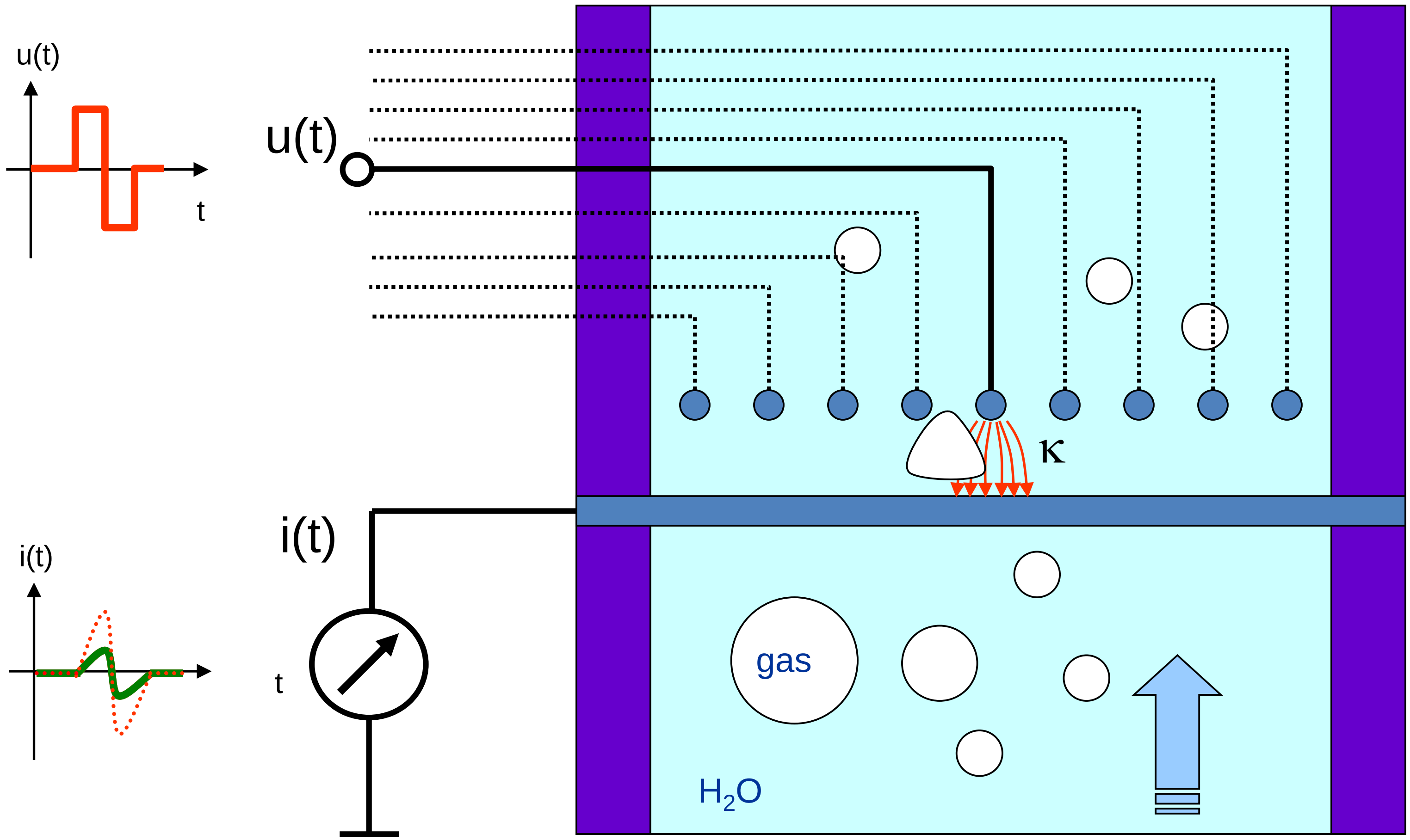
Wire-mesh Sensors



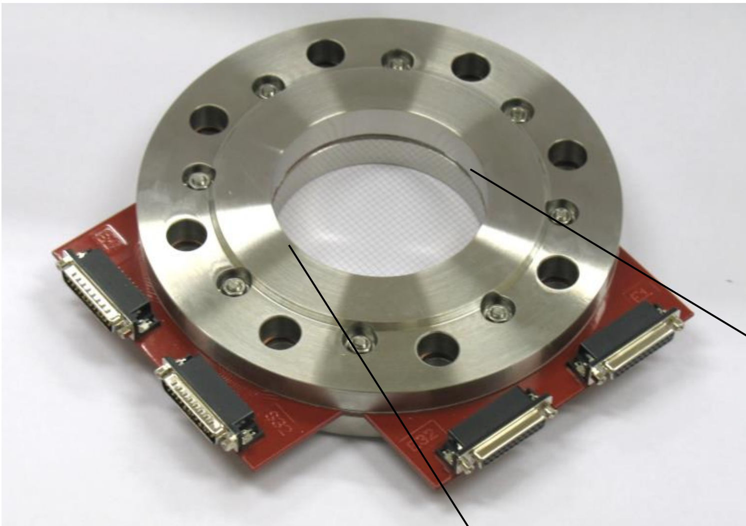
Wire-mesh Sensors

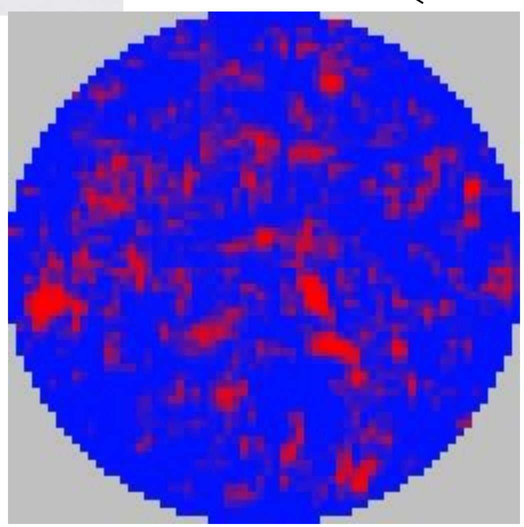


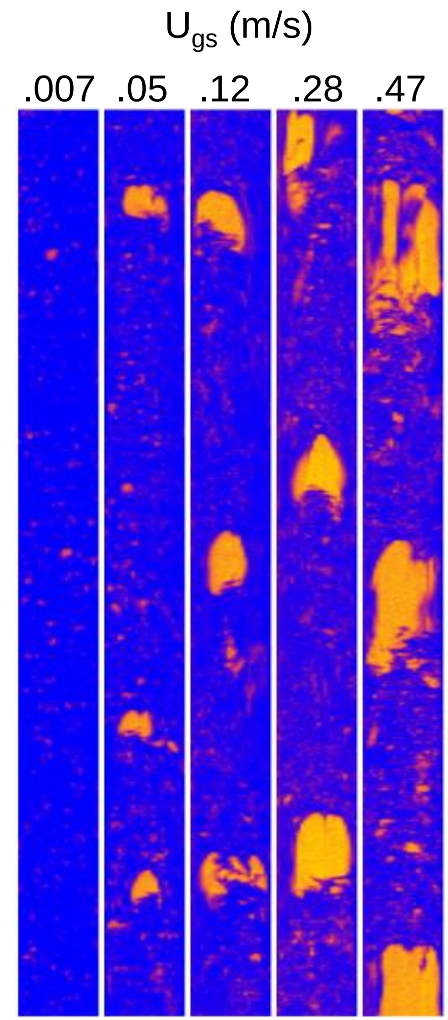
Wire-mesh Sensors



Wire-mesh Sensors





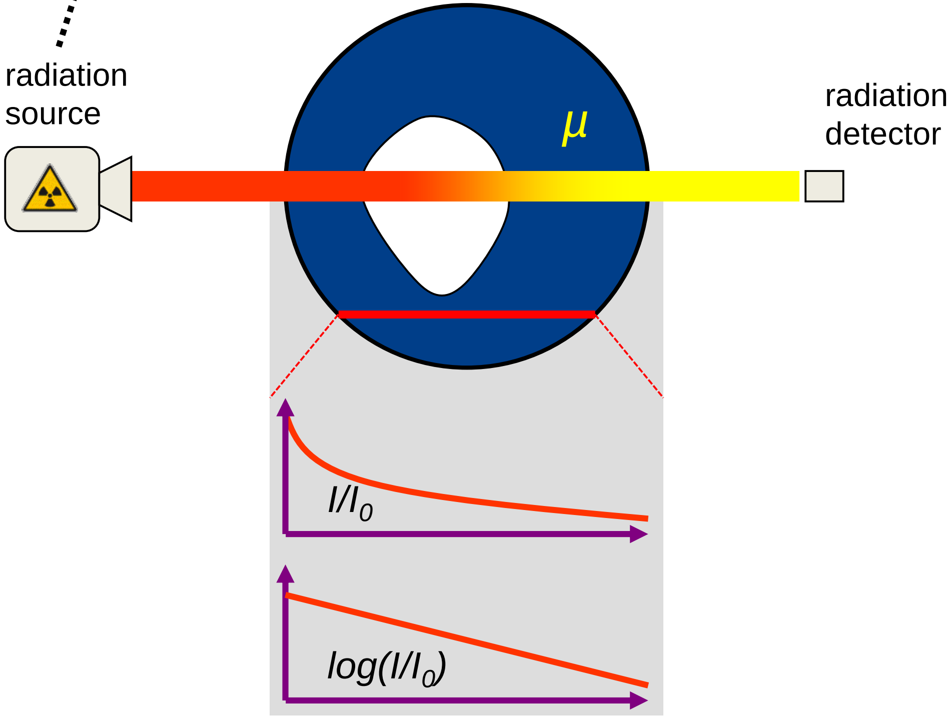


- Temporal resolution up to 10.000 fps
- Pipe diameter up to 200 mm
- Mixture velocities up to 10 m/s
- Wire mesh up to 64 x 64
- Spatial resolution up to 2 mm

Multiphase flow analysis with computed tomography

Computed Tomography

^{137}Cs
160 GBq
∅ ~5 mm



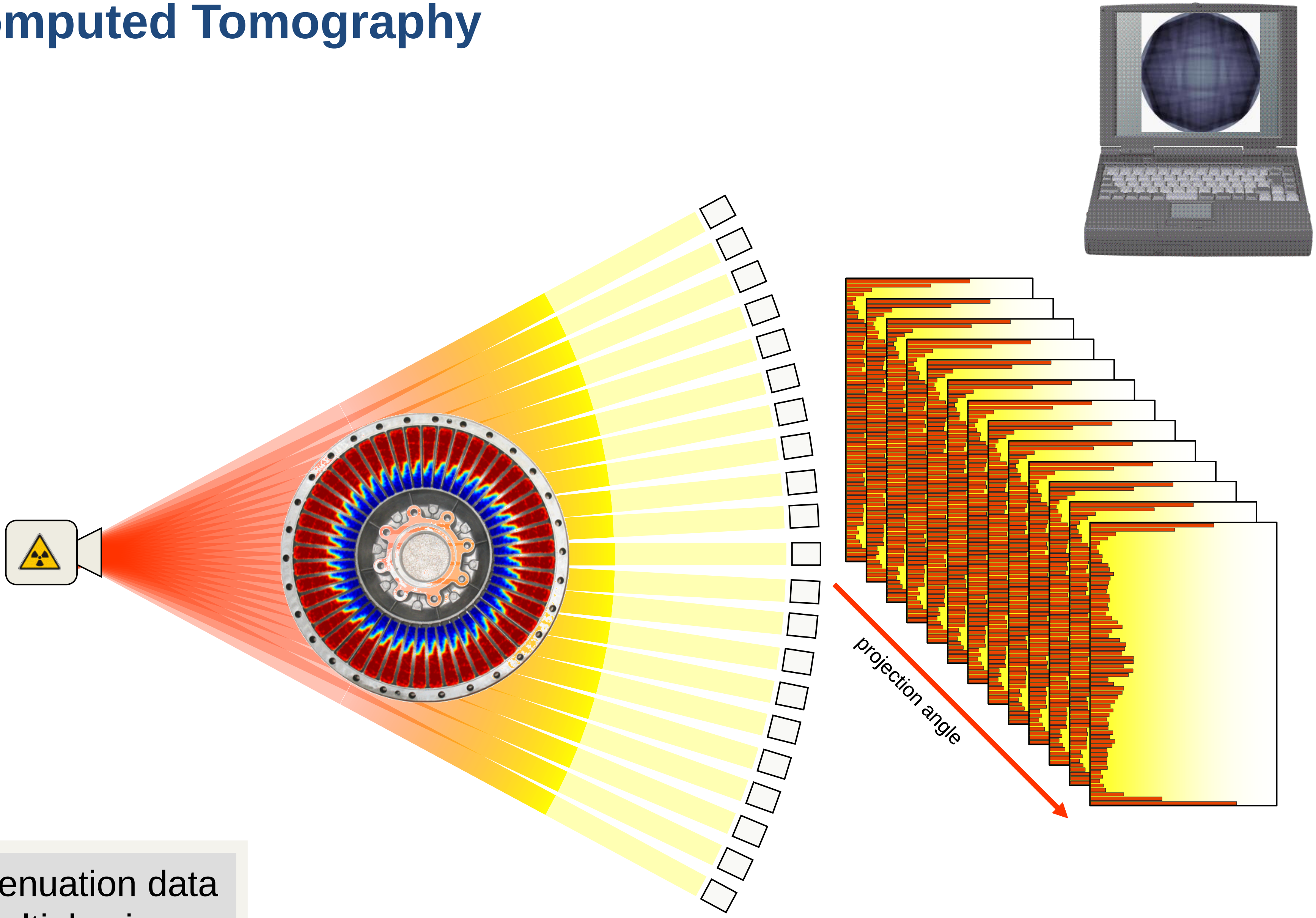
Radiation power is exponentially attenuated along the beam:

$$I = I_0 exp\left(-\int_Q^D \mu(s)ds\right)$$

The measurand E is a line integral of the attenuation coefficient μ

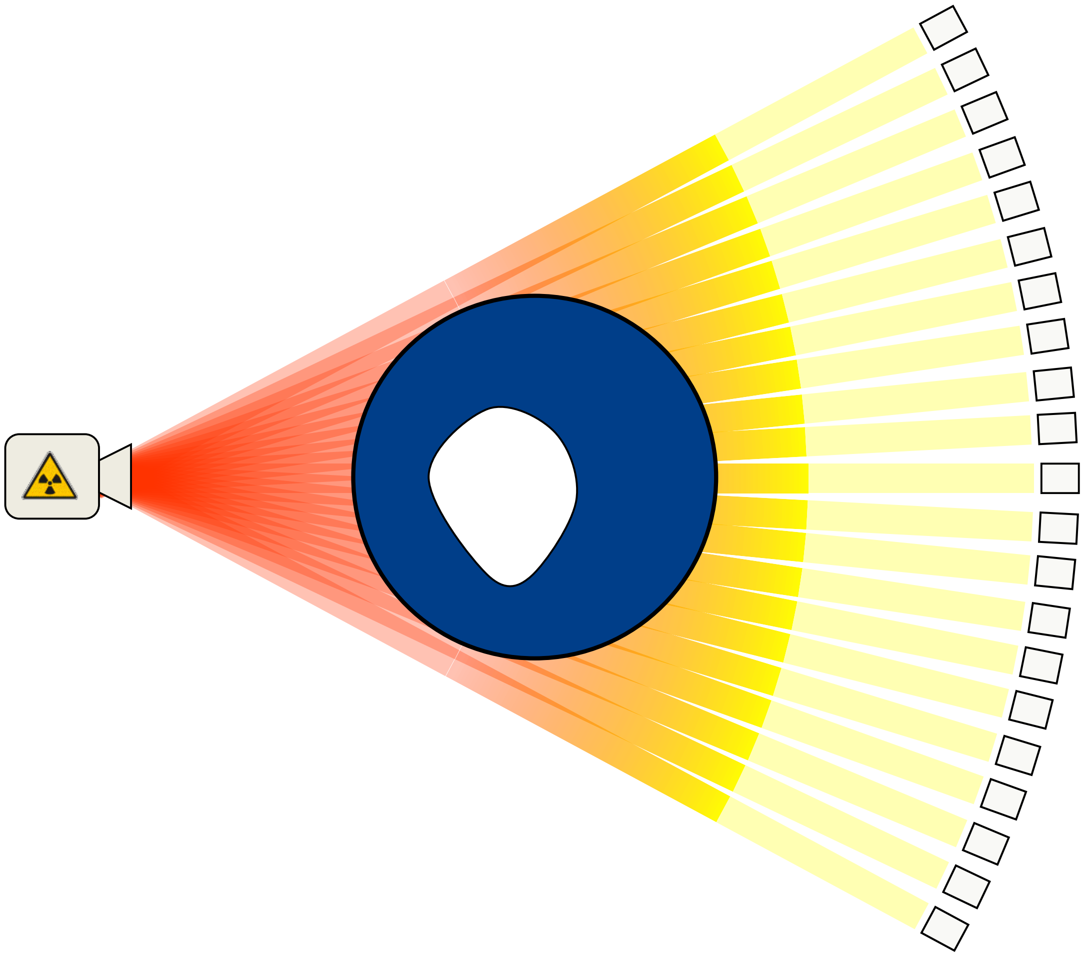
$$\mathrm{E} = -log\left(\frac{I}{I_0}\right) = \int_Q^D \mu(s)ds$$

Computed Tomography



Get attenuation data from multiple views

Ultrafast X-ray Computed Tomography

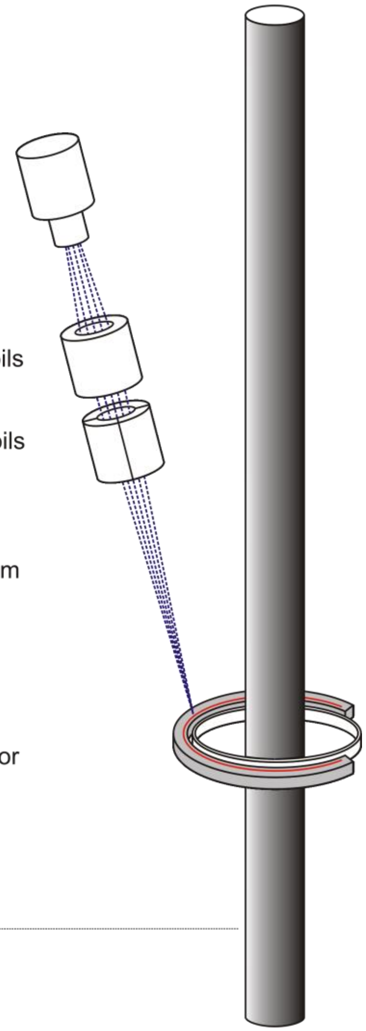


Tomography means
creeping around
your object!

Can it be made
fast enough to capture
transient flow details?

1000 frames/second =
1000 revolutions/second !

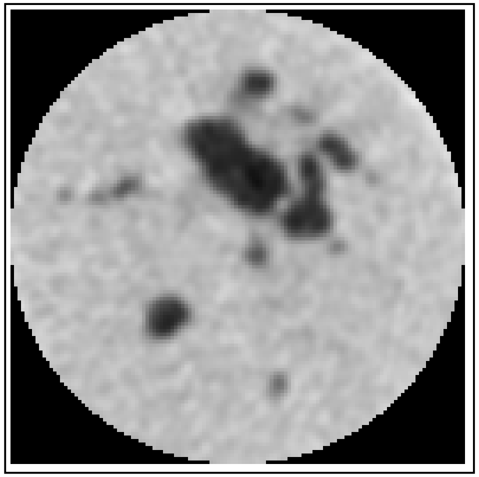
Ultrafast X-ray Computed Tomography

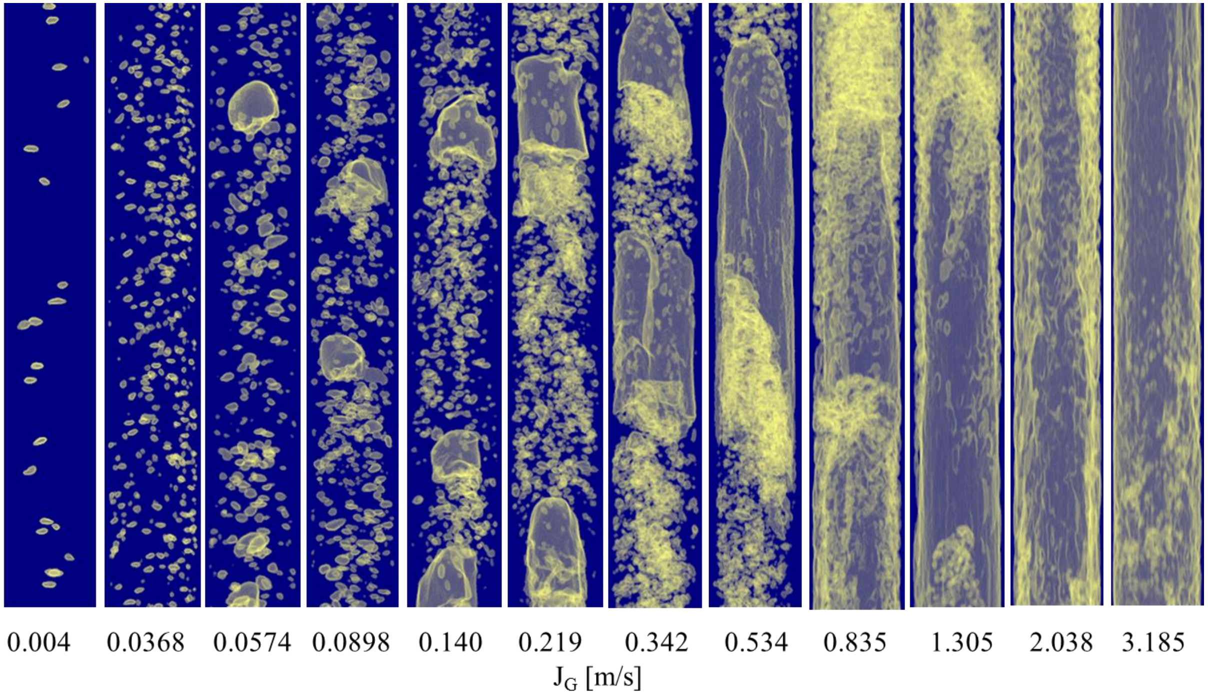


Fischer (2008)

Ultrafast X-ray Computed Tomography

∅50 mm, 1000 fps



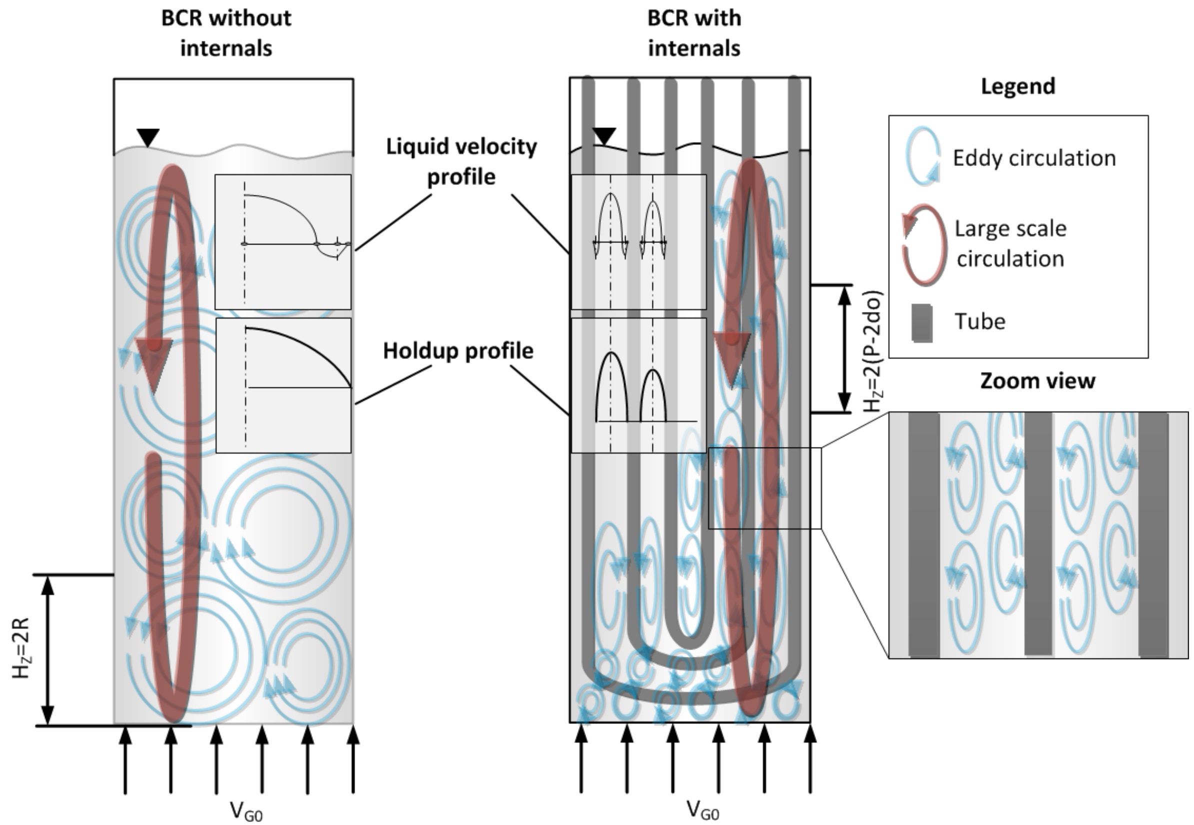


An application example

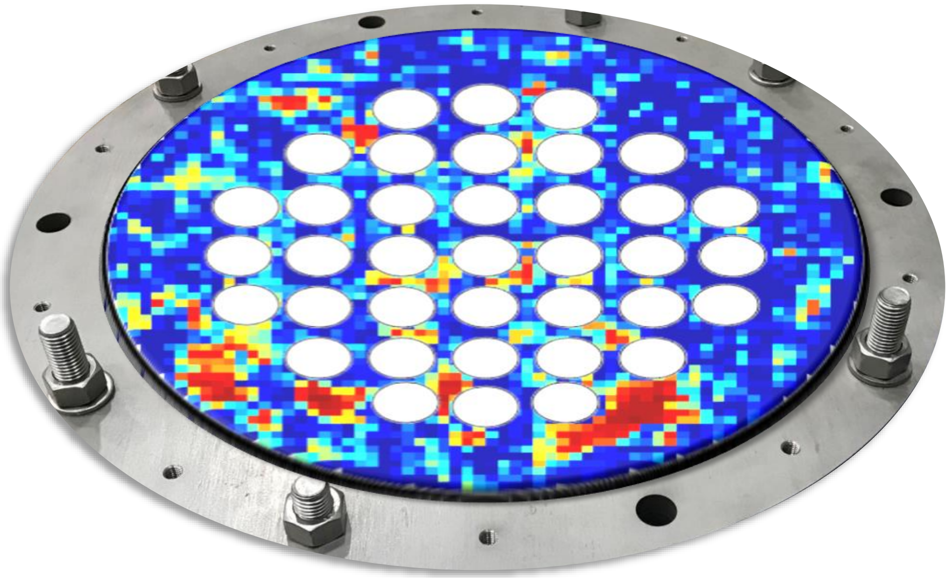
Bubble Column Reactors with Internals

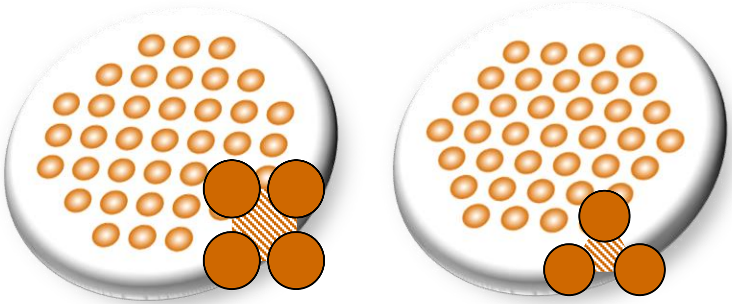
Process	ΔH_r (kJ/mol)	P (bar)	T (°C)
FT-Synthesis	-210	30-40	250-290
Methanol Synthesis	- 91	50-100	220-270

©Timmerman Heat Exchangers & Piping



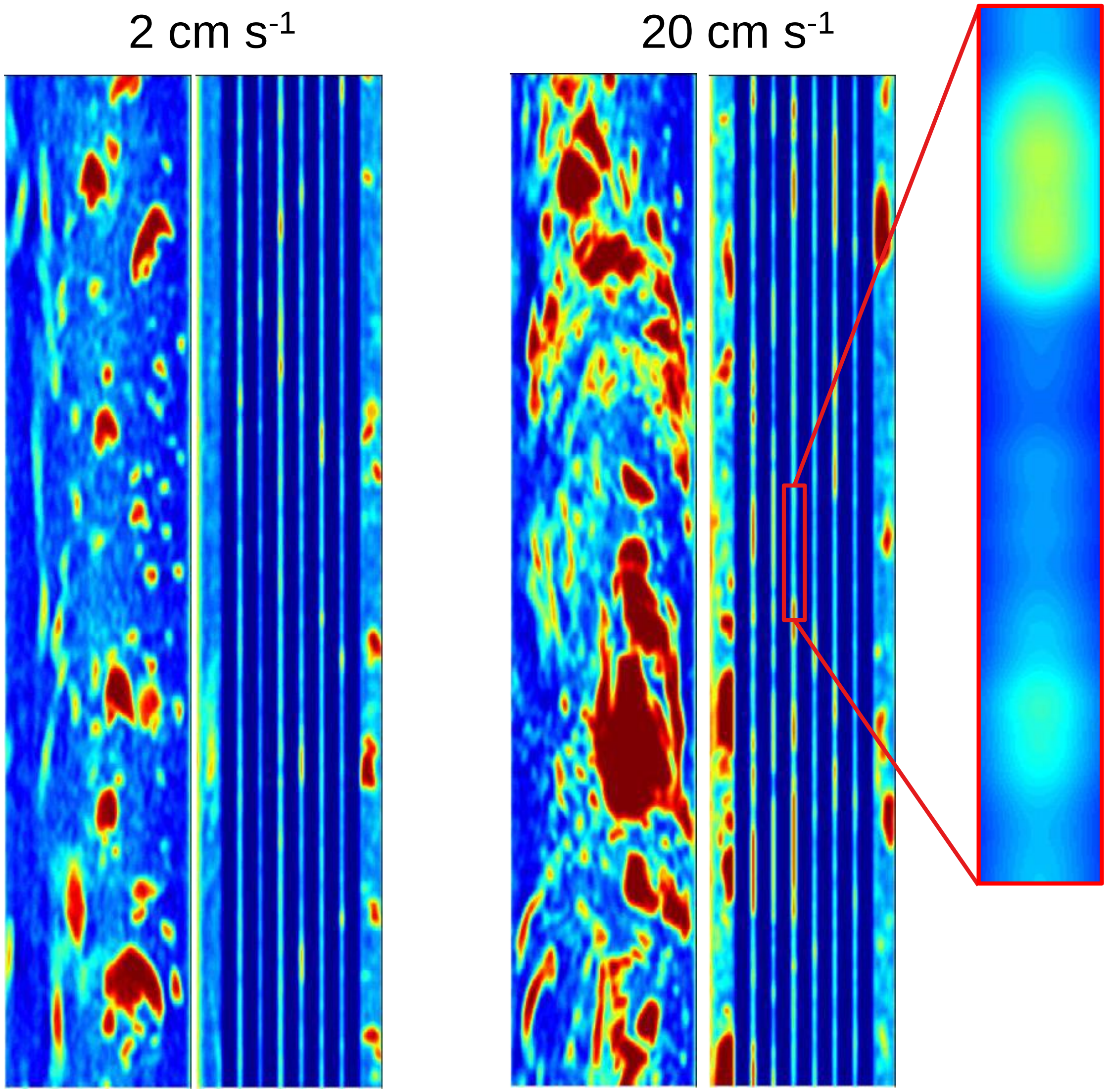
Bubble Column Reactors with Internals

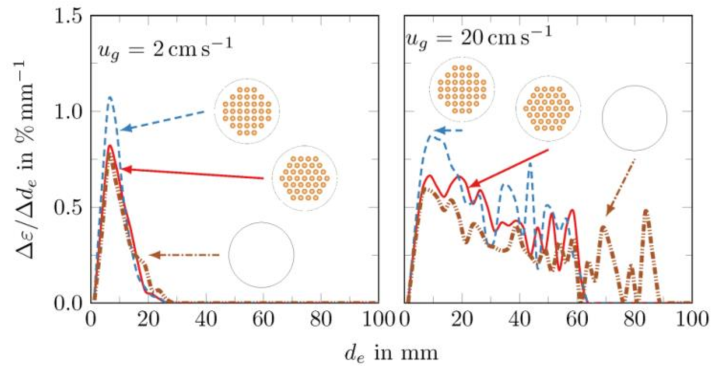




Bubble Column Reactors with Internals

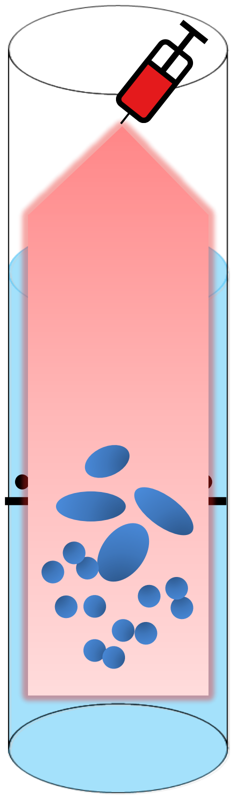
Obtaining the bubble size distribution

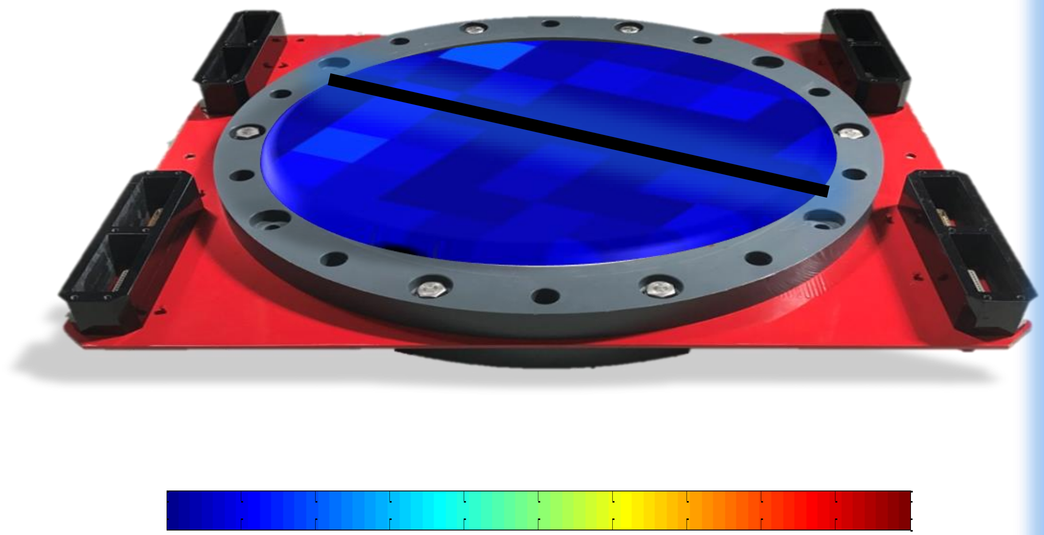




Bubble Column Reactors with Internals

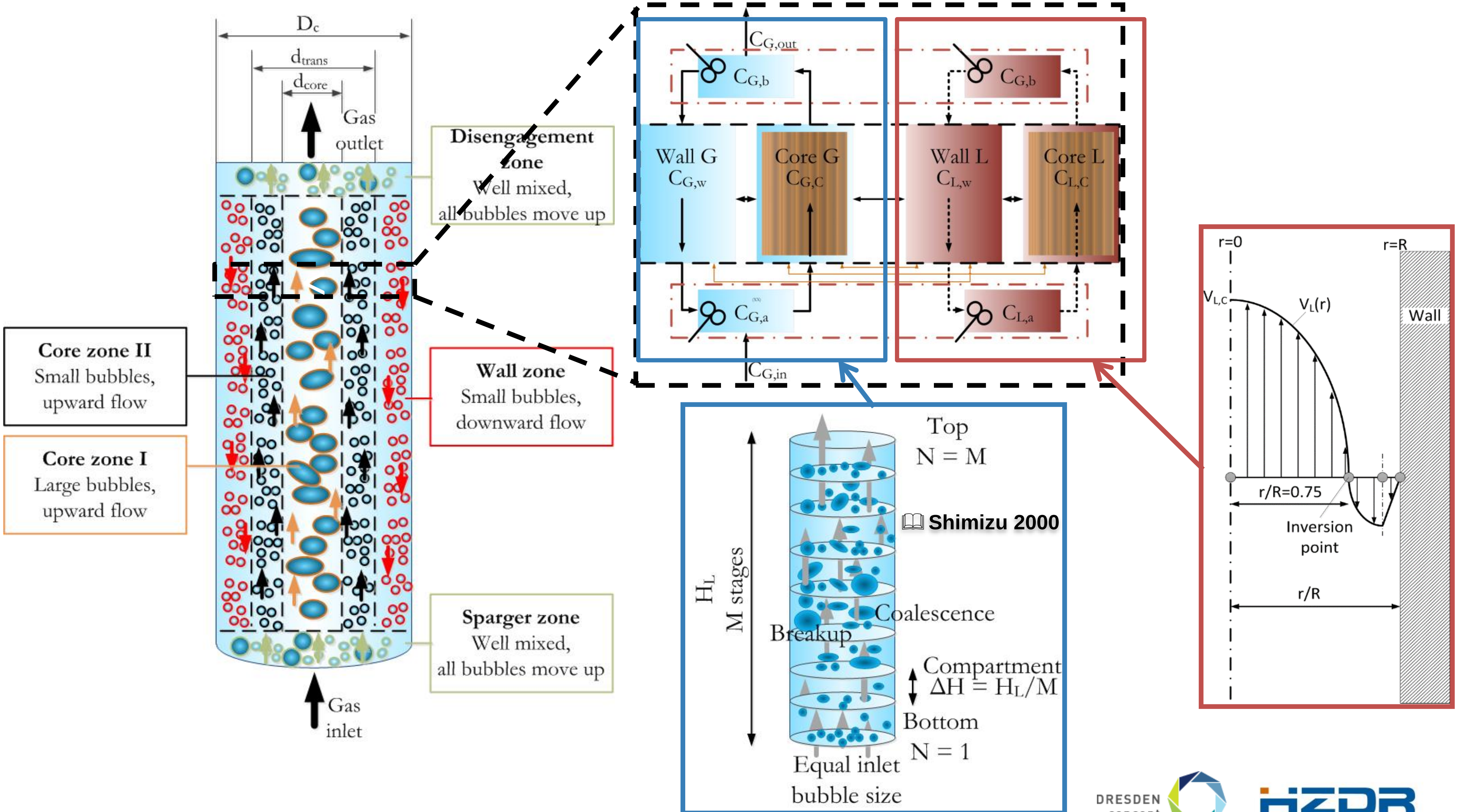
Obtaining the liquid velocity profile





Bubble Column Reactors with Internals

An advanced reactor model



DRESDEN concept

HZDR

Thank you for your attention